2.6 Propagators and Feynman Path integrals

REF: Gottfried and Yan Ch. 2.6, 2.7

(1) propagators

* Remark

These particular formulations of QM are used typically for the "many"-particle QM, but we just consider a single-particle case only, for the simplicity.

- Time evolution of a state $|\alpha\rangle$

$$\Rightarrow |\alpha, t_0; t\rangle = U(t,t_0)|\alpha, t_0\rangle$$

This is what we know.

and the Schödinger eq.

$$\Rightarrow \quad i\hbar\frac{\partial}{\partial t}U(t,t_0) = H(t)\,U(t,t_0)$$

← we also know this.

by multiplying $\langle \vec{x}_1|\cdot$, $t \to t_1$

$$\psi_\alpha(\vec{x}_1, t_1) = \int d^3x_0 \, \langle \vec{x}_1| U(t_1,t_0)|\vec{x}_0\rangle \, \psi_\alpha(\vec{x}_0, t_0)$$

: It moves the state both into the future and the past.

$\psi_\alpha(\vec{x},t) = \langle \vec{x}|\alpha, t\rangle$.

Choose the future:

$$\psi_\alpha(\vec{x}_1, t_1) = \int d^3x_0 \, K(\vec{x}_1 t_1, \vec{x}_0 t_0)\, \psi_\alpha(\vec{x}_0, t_0)$$

where ☆

$$K(\vec{x}_1 t_1, \vec{x}_0 t_0) = \langle \vec{x}_1|U(t_1,t_0)|\vec{x}_0\rangle \cdot \Theta(t_1 - t_0)$$

future!

⇒ It's a causal theory.

: time-evolution (unitary) of a wave function is deterministic.

→ Limiting behavior at $t_1 \to t_0$ $d=3$ in 3D.

$$\lim_{t_1\to t_0} K(\vec{x}_1 t_1, \vec{x}_0 t_0) = \delta^d(\vec{x}_1 - \vec{x}_0) \quad \Big\| \quad \because \lim_{t_1\to t_0} U(t_1,t_0) \to 1 .$$

→ Interpretation as a transition probability (amplitude)

$$K(\vec{x}_1 t_1, \vec{x}_0 t_0) = \langle \vec{x}_1, t_1 | \vec{x}_0, t_0 \rangle \quad \Big\| \quad |\vec{x}_0, t_0\rangle = |\vec{x}_0\rangle .$$

Composition property :

$$K(\vec{x}_2 t_2, \vec{x}_0 t_0) = \int d^3x_1\, K(\vec{x}_2 t_2, \vec{x}_1 t_1)\, K(\vec{x}_1 t_1, \vec{x}_0 t_0) .$$

$$(t_2 > t_1 > t_0) .$$

finding the system (particle) at $(\vec{x}_1, t_1)$, given that it was originally at $(\vec{x}_0, t_0)$.

→ How can we compute K ?

① If we know all E's and ψ's → trivial. (see below)

② One can get it directly from H :

$$\boxed{\left[i\hbar \frac{\partial}{\partial t} - H(\vec{x},t) \right] K(\vec{x}t, \vec{x}_0 t) = i\hbar\, \delta(t-t_0)\, \delta^d(\vec{x}-\vec{x}_0)} \quad ☆$$

... inhomogeneous part of the Schrödinger eq.

verification

$$i\hbar \frac{\partial}{\partial t} K = i\hbar \langle \vec{x} | \frac{\partial}{\partial t} U(t,t_0) | \vec{x}_0 \rangle \Theta(t-t_0)$$
$$+ i\hbar \langle \vec{x} | U(t,t_0) | \vec{x}_0 \rangle \delta(t-t_0) .$$
$$= \langle \vec{x} | H\, U(t,t_0) | \vec{x}_0 \rangle \Theta(t-t_0)$$
$$+ i\hbar \langle \vec{x} | \vec{x}_0 \rangle \delta(t-t_0) \quad \leftarrow \quad \lim_{t\to t_0} U(t,t_0) = 1$$
$$= H(\vec{x},t)\, K(\vec{x}t, \vec{x}_0 t_0)$$
$$+ i\hbar\, \delta(t-t_0)\, \delta^d(\vec{x}-\vec{x}_0) .$$

Note : "local" potential.

$$H(\vec{x},t) = \langle \vec{x} | H | \vec{x}' \rangle = H(\vec{x},t)\, \delta(\vec{x}-\vec{x}')$$

ex. $-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})$

$\to$ dimension of K ?

$$[\underbrace{i\hbar \partial_t - H}_{=\text{ energy } = [\hbar]T^{-1}}]K = i\hbar \underbrace{\delta(t-t_0)}_{\to T^{-1}} \underbrace{\delta^d(\vec{x}-\vec{x}_0)}_{\to L^{-d}}$$

$$\Rightarrow \quad [K] = L^{-d} \quad ☆$$

(2) Green's functions

☆ t-indep. $H \Rightarrow \mathcal{U}(t,t_0) = \exp\left[-\frac{i}{\hbar}H(t-t_0)\right]$

: time-evolution operator depends only on $t-t_0$!

$\to$ let $t-t_0 \equiv t$.

- propagator $K(\vec{x}_1,\vec{x}_0;t) \equiv \langle \vec{x}_1 | e^{-\frac{i}{\hbar}Ht} | \vec{x}_0\rangle \Theta(t)$

If we know all E_n's and $\{|n\rangle\}$,

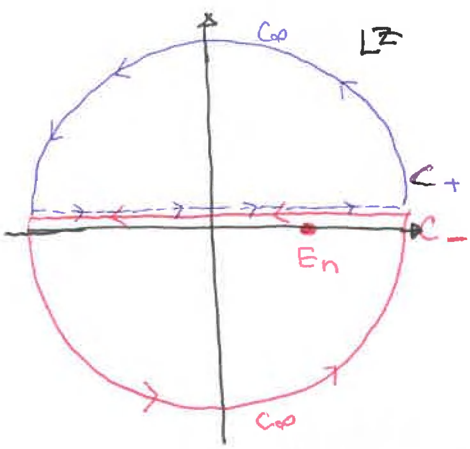
$$K(\vec{x}_1,\vec{x}_0;t) = \Theta(t)\sum_n e^{-\frac{i}{\hbar}E_n t}\, u_n(\vec{x}_1)\, u_n^*(\vec{x}_0)$$

$u_n(x) = \langle x|n\rangle$: energy eigenfunction

$\Rightarrow$ Integral representation

$$\boxed{K(\vec{x}_1,\vec{x}_0;t) = \frac{i}{2\pi}\int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} dz\, e^{-izt/\hbar}\sum_n \frac{u_n(\vec{x}_1)u_n^*(\vec{x}_0)}{z-E_n}}$$

Check : $\displaystyle\int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} dz\, e^{-izt/\hbar}\frac{1}{z-E_n}$



i) $t>0$

$$\int_{C_-} = -\int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} + \cancel{\int_{C_\infty}}^{\,0} = 2\pi i\, e^{-\frac{i}{\hbar}E_n t}$$

ii) $t<0$

$$\int_{C_+} = \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} + \cancel{\int_{C_\infty}}^{\,0} = 0 .$$

"no pole"

→ Green's function (inverse transformation)

$$G(\vec{x}_1, \vec{x}_0 ; E) = \frac{1}{i\hbar} \int_0^\infty dt\, e^{i(E+i\epsilon)t/\hbar} K(\vec{x}_1, \vec{x}_0 ; t)$$

$$= \sum_n \frac{u_n(\vec{x}_1)\, u_n^*(\vec{x}_0)}{E - E_n + i\epsilon}$$ //

- How to get it from H :

$$[E - H(\vec{x})]\, G(\vec{x}, \vec{x}_0 ; E)$$

$$= \sum_n \frac{[E - H(\vec{x})]\, u_n(\vec{x})\, u_n^*(\vec{x}_0)}{E - E_n + i\epsilon} = \sum_n u_n(\vec{x})\, u_n^*(\vec{x}_0)$$

$$= \delta^d(\vec{x} - \vec{x}_0)$$

$$\Rightarrow \boxed{\left(E - H(\vec{x})\right) G(\vec{x}, \vec{x}_0 ; E) = \delta^d(\vec{x} - \vec{x}_0)}$$

... inhomogeneous Schrödinger eq.
with a source term.

(3) Free particle K and G
... examples in "1D"

- No potential : $\mathcal{H} = \frac{1}{2m} \tilde{p}^2$

- free-particle propagator

$$K(x, x' ; t) = \langle x | \, \underbrace{\quad}_{\Sigma |p\rangle\langle p|} e^{-\frac{i \tilde{p}^2}{2m\hbar} t} \underbrace{\quad}_{\Sigma |p'\rangle\langle p'|} | x' \rangle\, \Theta(t) .$$

∗ H is translation invariant : We can just set $x' = 0$ //

$$\Rightarrow K(x, t) = \Theta(t) \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, e^{\frac{i}{\hbar}\left[px - \frac{p^2 t}{2m}\right]}$$

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}}$$

$$K(x,t) = \Theta(t) \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \exp\left[-\frac{it}{2m\hbar}\left(p - \frac{m}{t}x\right)^2 + i\frac{mx^2}{2\hbar t} \right]$$

→ just ~~Gaussian~~ Fresnel integration.

$$= \Theta(t) \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left[i\frac{mx^2}{2\hbar t} \right]$$

.... easy to generalize to 3D cases. // This is it.

$$\int_{-\infty}^{\infty} dx\, e^{\mp i|a|x^2} = \sqrt{\frac{\pi}{\pm i|a|}} = \begin{cases} \sqrt{\frac{\pi}{i|a|}} \\ \sqrt{\frac{\pi}{|a|}}\, i \end{cases}$$

- free-particle Green's function (3D)

$$(\nabla^2 + k^2)\, G(\vec{x}, k) = \delta(\vec{x})$$

→ Helmholtz eq. $\quad \| \quad k^2 = \frac{2mE}{\hbar^2}$

$$\Rightarrow \quad G_{ret}(\vec{x}, k) = -\frac{1}{4\pi}\frac{e^{ikr}}{r}$$

"retarded" : outgoing. $(E \to E + i\epsilon)$ (going to the future) $\updownarrow$ $t > 0$.)

c.f.) If we set $E \to E - i\epsilon$ $(t<0)$

$$G_{adv}(\vec{x}, k) = -\frac{1}{4\pi}\frac{e^{-ikr}}{r} \quad \text{(incoming)}$$

"advanced" (coming back to the past).

(4) Perturbation Theory *

... This is what all these things are about.

$$H = H_0 + V$$

↳ Suppose that we know K_0 and G_0.

- propagator.

for H :

$$1 \leftarrow 2$$

$$[i\hbar\partial_t - H_0]\, K(x_1t_1, x_2t_2)$$

$$= V(x_1t_1)\, K(x_1t_1, x_2t_2) + i\hbar\,\delta^d(x_1 - x_2)\,\delta(t_1 - t_2)$$

for H_0 :

$$[i\hbar\partial_t - H_0]\, K_0(x_1t_1, x_2t_2) = i\hbar\,\delta^d(x_1 - x_2)\,\delta(t_1 - t_2)$$

$$\Rightarrow \left[i\hbar\partial_t - H_0\right]\Big(K(x_1t_1, x_2t_2) - K_0(x_1t_1, x_2t_2)\Big)$$

$$= V(x_1t_1)\, K(x_1t_1, x_2t_2)$$

$$\overset{\exists}{\Rightarrow}\ K(x_1t_1, x_2t_2) = K_0(x_1t_1, x_2t_2)$$

$$+ \frac{1}{i\hbar}\int dx_3\, dt_3\, K_0(x_1t_1, x_3t_3)\, V(x_3t_3)\, K(x_3t_3, x_2t_2)$$

Let $1 \equiv (x_1t_1)$, $2 \equiv (x_2t_2)$, $3 \equiv (x_3t_3)$

$$K(1,2) = K_0(1,2) + \frac{1}{i\hbar}\int d3\, K_0(1,3)\, V(3)\, K(3,2)$$

perturbation expansion.

$$\Rightarrow K(1,2) = K_0(1,2) + \frac{1}{i\hbar}\int d3\, K_0(1,3)\, V(3)\, K_0(3,2)$$

$$+ \left(\frac{1}{i\hbar}\right)^2\int d3\, d4\, K_0(1,3)\, V(3)\, K_0(3,4)\, V(4)\, K_0(4,2)$$

$$+ \left(\frac{1}{i\hbar}\right)^3 \cdots + \left(\frac{1}{i\hbar}\right)^4 \cdots$$

- Green's function.

$\rightarrow$ Its operator consists the resolvent.

projection op.

def. $$\mathcal{G}(z) \equiv \frac{1}{z-H} = \sum_n |n\rangle \frac{1}{z-E_n}\langle n| = \sum_n \frac{P_n}{z-E_n}$$

$\rightarrow$ Green's function

$$G(\vec{x}, \vec{x}'; E) = \langle \vec{x}|\, \mathcal{G}(E+i\epsilon)\, |\vec{x}'\rangle$$

Schrödinger eq.

$$(z-H)\,\mathcal{G}(z) = \mathbb{1}$$

$$(E-H)\, G(\vec{x}, \vec{x}'; E) = \delta(\vec{x}-\vec{x}')$$

well-defined
as long as z is not on the real axis.

now, $\underline{H = H_0 + V}$ vs $\underline{H_0}$

$$\Rightarrow \mathcal{G}(z) = \frac{1}{z - H_0 - V} \quad \text{vs} \quad \mathcal{G}_0(z) = \frac{1}{z - H_0}.$$

By using the identity, $\frac{1}{A-B} = \frac{1}{A} + \frac{1}{A} B \frac{1}{A-B}$

$$= \frac{1}{A} + \frac{1}{A-B} B \frac{1}{A}$$

$$\Rightarrow \mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 V \mathcal{G} \quad // \quad A \equiv z - H_0, \; B \equiv V$$

!

$$\hookrightarrow \mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 V \mathcal{G}_0 + \mathcal{G}_0 V \mathcal{G}_0 V \mathcal{G}_0 + \cdots$$

… Born series "

$\Rightarrow$ Integral equation for the Green's function.

$$G(\vec{x}, \vec{x}') = G_0(\vec{x}, \vec{x}') + \int d\vec{s}\; G_0(\vec{x}, \vec{s})\, V(\vec{s})\, G(\vec{s}, \vec{x}')$$

// E is omitted.

(5) The Feynman Path Integral. "

Dirac: $\exp\left[\frac{i}{\hbar} \overbrace{\int_{t_1}^{t_2} dt\, L_{\text{classical}}}^{= S \text{ (classical action)}}\right]$ corresponds to $\langle x_2 t_2 | x_1 t_1 \rangle$.

???

Feynman: $\exp\left[\frac{i}{\hbar} S\right]$ is proportional to $\langle x_2 t_2 | x_1 t_1 \rangle$.

!

path integral

$$\Rightarrow \langle x_N t_N | x_1 t_1 \rangle = \int_{x_1}^{x_N} \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} S[x(t)]}.$$